

All data taken at Pacific Northwest National Laboratory (PNNL)
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Composite spectrum for DEFAMD_50T

Effective burden of composite spectrum: 1 part-per-million-meter (ppm-meter) at 296 K

Equivalent concentration x path-length of composite spectrum: 4.1643×10^{-6} grams/liter-meter

Sample Conditions-

- Chemical name and CAS number: N,N-Diethyl formamide; Formamide, N,N-diethyl-; Diethylformamide; N-Formyldiethylamine; $C_5H_{11}NO$: [617-84-5]
- Physical properties: MW=101.1470 g/mole, mp=n/a° C, bp=177.6° C, Density (25 C) = 0.908 g/cm³
- Supplier and stated purity: Sigma Aldrich, 99%
- Sample class: I (PNNL scale).
- Temperature of White cell (805.0 cm optical path length) 50 ± 2 C
- Diluent (high purity nitrogen) flowed at 23.3 liter/min (21.1° C), ambient atmospheric pressure 760 ± 5 Torr.
- Samples flowed at microliters/minute 5.000, 2.000, 10.000, 17.500, 7.500, 3.500, 12.500, 25.000, 6.250, 35.000, 15.000, 21.000, 8.750 and 30.000.
- Individual samples at equivalent pressures of: 0.035016, 0.014008, 0.070050, 0.122603, 0.052537, 0.024517, 0.087574, 0.175171, 0.043816, 0.245435, 0.105186, 0.147280, 0.061367 and 0.210428 Torr. Final data is a composite spectrum.
- Preparation: None

Instrument Parameters-

- Bruker-66V FTIR, evacuated optics bench.
- Modified to include second aperture, between interferometer output and White cell. This substantially reduces both “ghosting” and warm aperture effects.
- Spectral range: 6,500 to 520 cm⁻¹ (1.538 to 19.23 microns)
- Instrumental resolution based on maximum interferometer displacement is 0.112 cm⁻¹
- Spectral interval after 2X zero-filling interferogram and FFT: 0.06 cm⁻¹
- Interferogram zero-fill: 2X
- Apodization: Boxcar
- Phase correction: Mertz
- Beam splitter: Potassium bromide (KBr)
- IR source: Carbide glowbar (22 V)
- Scanner velocity: 60KHz (HeNe crossing frequency)
- Number of interferograms averaged per single channel spectra: 256
- Detector: Mid-band HgCdTe, photoconductive, 77K operation
- Folding limits: 15798 to 0 cm⁻¹

Post Processing and Related Parameters-

- Non-linearity detector correction (Bruker proprietary) applied to interferogram ($\alpha=0.90$, $\epsilon=500$)
- Composite spectrum created from 14 individual absorbance (base-10) spectra via classical least squares fit: Intercept=0, slope is fitted, individual absorbance values weighted by T² (transmission squared), all absorbance values ≥ 1.6 are given zero weight

- Calculated and estimated errors: Type A =0.72%, Type B \leq 7%
- Frequency correction (already applied): $V(\text{corrected})=V(\text{instrument})\cdot 0.9999996+6.17682\times 10^{-4}$
- Axis units: X=wavenumbers (cm^{-1}), Y=Absorbance (base-10)
- Trace water vapor and carbon dioxide were removed by spectral subtraction
- Baseline correction via 7th order polynomial subtraction